

The external perturbations can be temperature, light irradiation, pressure, and pulsed magnetic fields all may change the magnetic coupling interaction in transition metal systems. Here, we use pressure as external force to study magneto-structural correlation.

We report here the structure and magnetic behavior of one 1-D helical chain iron complex $[\text{FeII}(\mu\text{-bpt})(\mu\text{-COOC}_5\text{H}_4\text{N}) \cdot 1/2 \text{H}_2\text{O}]_n$ (bpt=3,5-bis (pyrid-2-yl)-1,2,4-triazole), [1], in ambient conditions and under hydrostatic pressure. The complex was crystallized in a tetragonal space group $I4_1/a$ at ambient pressure, each iron atoms linked by one bpt and one isonicotinic acid legend, which form an infinite helical chain along the screw axis 4_1 at c-axis direction. The iron atoms are iron (2+) high spin state with distorted N_4O_2 coordinated shell.

High-pressure powder X-ray diffraction experiments from 0.03GPa to 2.79GPa pressure were carried out to understand precisely the correlation between the structure and magnetic behavior. The careful analysis of a series high pressure structures showing a pressure-induced shrinking more than 10% along the chain direction, which can describe as spring compressed 10%. This make the iron-iron distance from 4.445(2) Å at ambient pressure change significantly to 4.083(6) Å at around 2GPa. Magneto-structural correlation will be discussed. The coordinated shells of Iron (N_4O_2) also decrease 0.11 Å about averagely. The spin state of iron and magnetic property of title compound also will be shown in this report

[1] S-M Chen, *Structure and Magnetic Properties of Dinuclear metal Complexes with a Tetradentate bpt Ligand*. Ph. D. Thesis, 2009, National Taiwan University, Taipei, Taiwan. R.O.C.

Keywords: high pressure XRD, molecular magnetic materials, high pressure magnetism

MS20.P01

Acta Cryst. (2011) A67, C332

Structure and OD character of $5M_3$ ferriphlogopite from Ruiz Peak

Massimo Nespolo, Isabella Pignatelli, CRM2 UMR CNRS 7036, Institut Jean Barriol, Nancy-Université, Vandœuvre-lès-Nancy (France). E-mail: massimo.nespolo@crm2.uhp-nancy.fr

The first finding of a non-MDO mica polytype where two types of layers coexist is here reported. The sample is a 5-layer ferriphlogopite from Ruiz Peak, New Mexico, crystallizing in $C2$, $a = 5.3146(2)$ Å, $b = 9.2063(3)$ Å, $c = 49.730(2)$ Å, $\beta = 92.031(4)^\circ$. Data collection was performed on a Mar345 equipped with image plate detector, with completeness of 99.4% up to resolution 0.8 Å, 5049 unique reflections of which 3195 observed, and redundancy 13.6. The homo-octahedral stacking sequence was determined by PID analysis [1] and corresponds to the $5M_3$ polytype [2]. The structure model was obtained from the atomic coordinates of the $1M$ polytype by applying the stacking vectors, and refined with Jana2006 [3], to $R_{\text{(obs)}} = 7.03\%$. A reliable model for the distribution of the octahedral cations (Mg^{2+} , Al^{3+} , Fe^{3+} , Ti^{4+}) in the 9 independent sites cannot be obtained by structure refinement; the occupation of these sites has instead been estimated by exploiting the OD nature of mica polytypes [4]. An iterative computation of the Fourier map from a hybrid data set including computed family diffractions ($k = 3n$), which correspond to the family structure in which all octahedral site have the same content, and observed non-family diffractions, followed by adjustment of the model to reproduce the computed map, has been performed; this unambiguously resulted in two layers out of three having a prominent peak in a *cis* site, all the layers being meso-octahedral. The OD symbol for this polytype is $|1.5\ 5.3\ 5.5\ 1.1\ 3.1|$.

The $5M_3$ polytype with all layer of type $M1$ (origin of the octahedral sheet in the *trans* site) belongs to the $3T$ structural series. In this

case, however, the presence of $M2$ layers testifies the occurrence of structural adjustments at the polytype formations stage [5]. The original components could have been a two equal basic structures ($1M$ or $2M_1$) differently oriented, or two different basic structures ($1M$ or $2M_1$ or $3T$). The possible formation mechanism is currently under investigation.

[1] H. Takeda, *Acta Crystallogr.* **1967**, 22, 845-853. [2] H. Takeda, Ross M., *Am. Mineral.* **1975**, 80, 715-724. [3] V. Petricek, M. Dusek, L. Palatinus, *Jana 2006. The crystallographic computing system* **2006**. [4] K. Dornberger-Schiff, K.O. Backhaus, S. Đurovič, *Clays Clay Minerals* **1982**, 30, 364-374. [5] M. Nespolo, *Clays Clay Minerals* **2001**, 49, 1-23.

Keywords: mica, OD, polytypism

MS20.P02

Acta Cryst. (2011) A67, C332

Euclidean groups in spaces of arbitrary dimensions

Vojtěch Kopský Department of theoretical physics, Institute of Physics, Czech Academy of sciences, Praha (Czech Republic) E-mail: kopsky@centrum.cz

Different categories of Euclidean groups are established according to an analysis of the Fundamental theorem on Euclidean groups which is formulated and proved. The first division is into the *space*, *subperiodic* and *site point groups*. According to the character of the translation subgroup, the groups with the *discrete*, *continuous* and *semicontinuous* lattice are distinguished. The groups are classified as the *crystallographic*, *noncrystallographic* and *partially crystallographic* groups. In this connection, the concepts of crystallographic and space groups are amended.

Geometric classes and their splitting into arithmetic classes are defined as usual. Arithmetic classes are the natural classification units and the groups of such a class are distinguished by systems of nonprimitive translations in Seitz symbols for Euclidean operators. If the geometric class is reducible (irreducible) then the arithmetic class is either reducible or decomposable (irreducible). The factorization of the groups of decomposable or reducible classes by partial translation subgroups leads to groups of lower dimensions of the translation subgroup.

The class of the systems of nonprimitive translations which differ only by shift functions define an *extension class* within which the groups differ only by their location. Groups of the extension class have the same Hermann-Mauguin symbol and the same symmetry diagram. It is shown how to take the group location into consideration which is not done in Vol. A of IT. As a result, the data about subgroups are incomplete. The location of groups has been first considered in Vol. E of IT and in a software attachment GI * KoBo-1 to Vol. D of IT.

Diagrams of the Young type are suggested for a rough classification of groups in arbitrary dimensions. The groups up to three dimensions are considered in detail as the groups of material physics and a unique system of Hermann-Mauguin symbols for them is developed.

Keywords: seitz symbols, extension class, group location

MS20.P03

Acta Cryst. (2011) A67, C332-C333

3D space groups 2D hyperbolic orbifolds and “sponge” groups

Stephen T. Hyde, Stuart Ramsden, Vanessa Robins. Department of Applied Mathematics, Research School of Physics, Australian National University, Canberra (Australia). E-mail: stephen.hyde@anu.edu.au